

2,2,4-Trimethyl-1,3-pentanediol
144-19-4 | DTXSID8027113

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 5.32 days

Global applicability domain: Inside

Local applicability domain index: 4.51e-01

Confidence level: 8.64e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Propylbenzene</div> <div>Measured: 24.3</div> <div>Predicted: 4.02</div>	<div>Image not found</div> <div>Ethylbenzene</div> <div>Measured: 120</div> <div>Predicted: 6.21</div>	<div>Image not found</div> <div>4-Ethyltoluene</div> <div>Measured: 24.3</div> <div>Predicted: 3.95</div>
<div>Image not found</div> <div>1,3-Diethylbenzene</div> <div>Measured: 88.3</div> <div>Predicted: 5.36</div>	<div>Image not found</div> <div>1,2-Dimethyl-4-ethylbenzene</div> <div>Measured: 40.7</div> <div>Predicted: 4.08</div>	